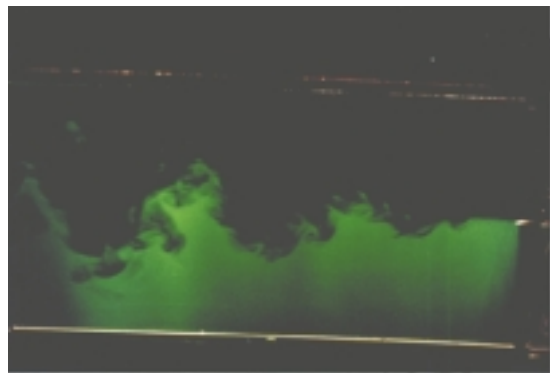




Theoretical Division

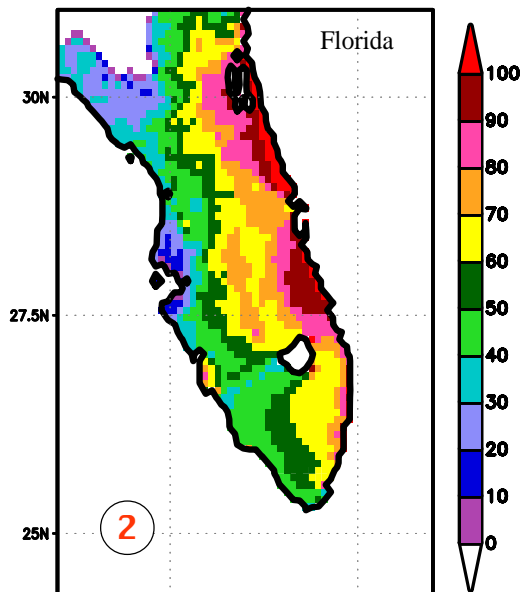
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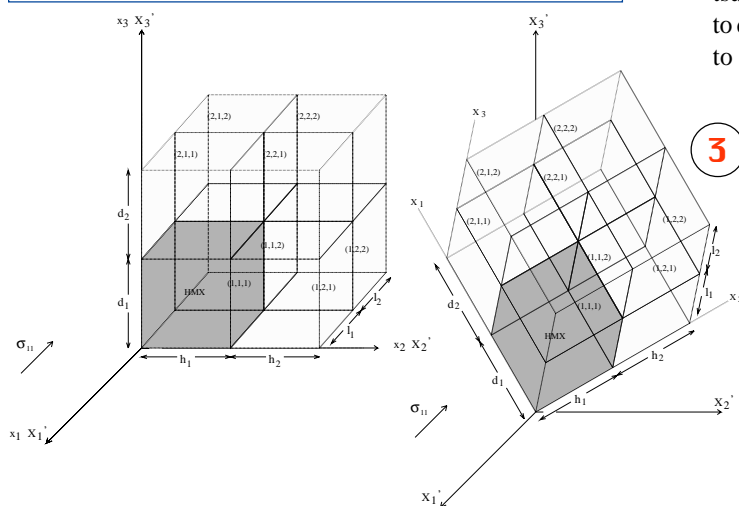
Spectral Nonequilibrium Turbulent Mixing Layer:

Experiments are performed in a water channel with two superimposed streams of different density entering at the same velocity above and below a splitter plate. Reproducible results show significant growth and decay of spectral anomalies before the spectral form reaches self-similar equilibrium downstream. Many of the nonequilibrium features are well represented with a turbulence model developed in T Division.



Tsunami from Asteroid-Comet Impact Deadly:

Impacts of large asteroid or comets into an ocean basin produce large tsunami runups along the shores of the entire basin. The tsunami from a large impactor (10 km) covers the coastal areas to depths exceeding 100 meters, and it even covers central Florida to a depth exceeding 60 meters.



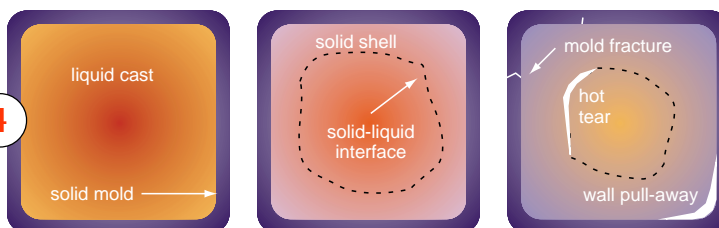
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Composite Materials Research:

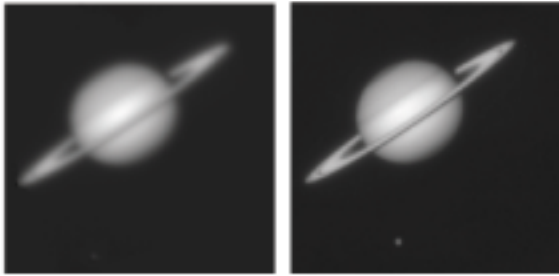
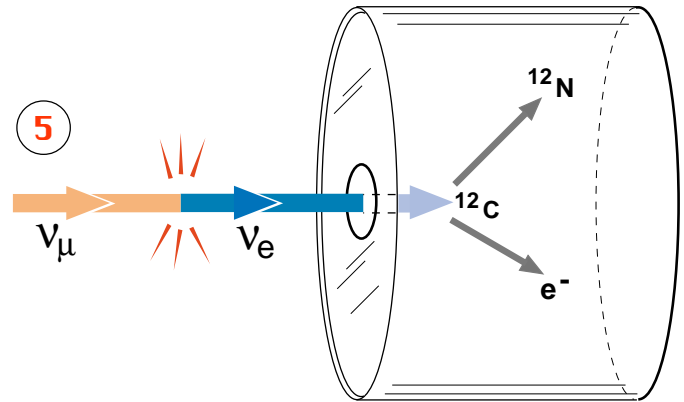
The field of composite material research is progressing rapidly due to increasing technological impetus; the economic gains are potentially great for possessing the capability to tailor materials with desired properties. Understanding the interrelationship between microstructure and material properties is important not only because of the necessity to develop methods for designing new materials but also because of scientific insight gained into the behavior of materials.

Solids in Alloy Casting Processes: As part of the plutonium-pit-rebuild program, casting technologies support manufacturing needs for stockpiled weapons systems. The casting process begins with molten alloy free-surface fluid flow, proceeds through cooling and solidification, and ends with a gradual cooling of the solid to ambient temperature. These coupled physical processes are being modeled using a simulation tool known as Telluride.

4

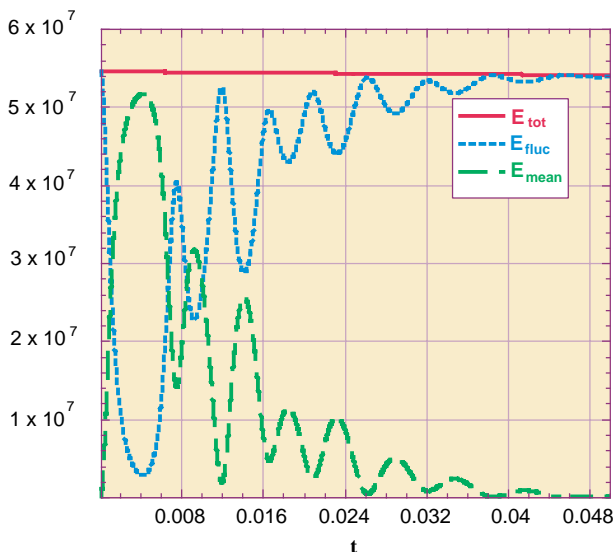
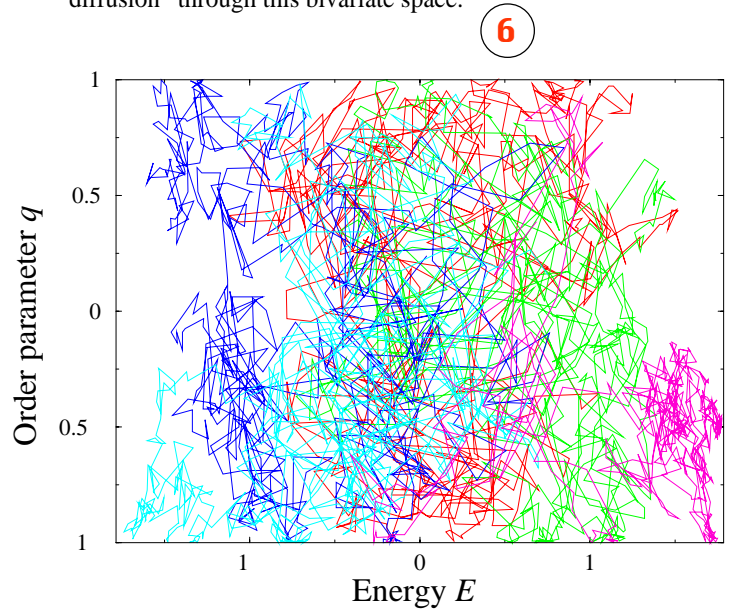


Neutrino Engineering: Oscillations of neutrinos from one type to another require that neutrinos have mass and that there exists new physics beyond the standard model of particle physics. One of the largest neutrino detectors uses a 52,000-gallon tank of mineral oil. Calculated cross sections for neutrino scattering from carbon in the oil provide crucial checks on the oscillation signals.



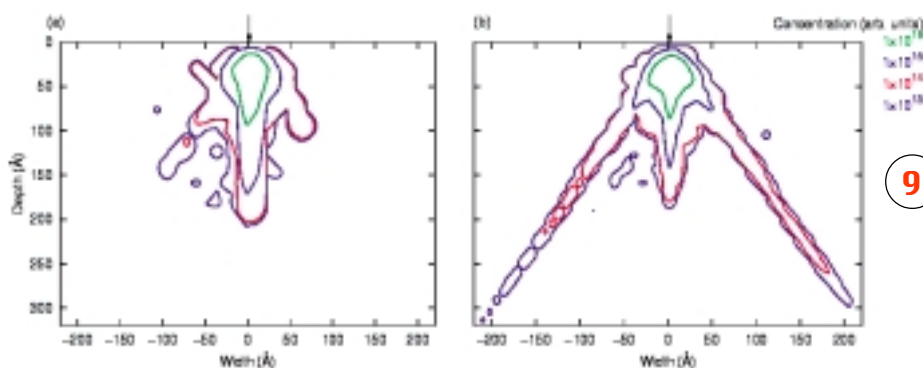
Modelling Artificial Guide Stars: Photons from laser-excited "artificial guide stars" are being used to greatly improve astronomical images. We have successfully modelled and predicted photon fluxes and other quantities measured in various experiments, and our simulations are being used in designs for adaptive optical systems employing artificial guide stars based on laser-excited mesospheric sodium.

Bivariate Multicanonical Monte Carlo of the $\pm J$ Ising Glass: A random walk in the space of allowable values of the energy and order parameter for a bivariate multicanonical simulation of a three-dimensional Ising glass. The path changes color after every 500 Monte Carlo steps to show the "diffusion" through this bivariate space.



Interactions of Fluid Turbulence and Mean Flow:

Parity-violating turbulence generates a mean flow in a bounded free-slip channel. In some cases, when the mean flow energy to turbulent energy is substantial, the spectral coefficients at two integer wave numbers m_y and m_y' become correlated in only a few bands of the form $m_y = \pm m_y' \pm |n|$, where y points in the inhomogeneous direction.



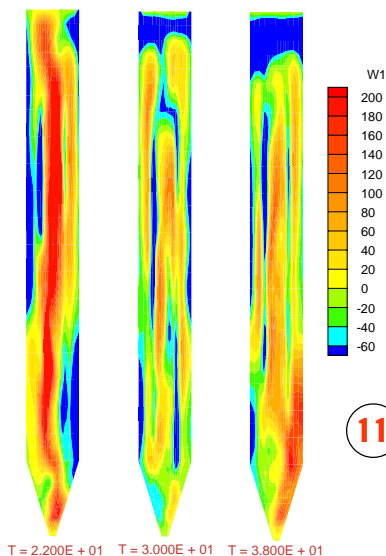
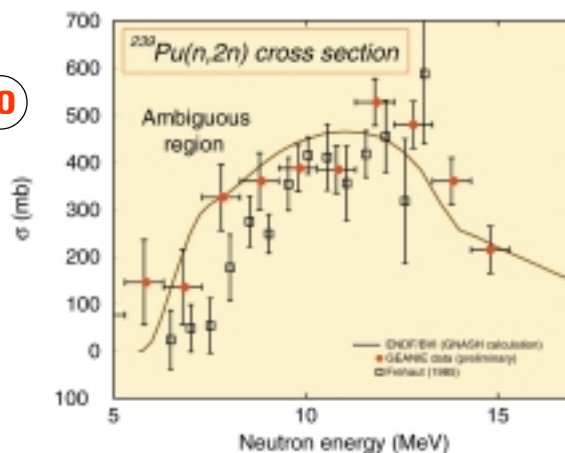
REED-MD Ion Implant

Simulator: A highly efficient molecular dynamics code to calculate concentration profiles of dopants implanted in semiconductors. 2D dopant profiles from 2 keV. As implant into Si {100}, with (a) 5 and (b) 15 angstroms of surface oxide. Greater surface disorder leads to more ions being scattered into the larger <110> channels, and hence gives a deeper profile.

Plutonium Reaction for Science-Based Stockpile Stewardship

The $^{239}\text{Pu}(n,2n)$ reaction is an important radiochemical detector for understanding the neutron fluence spectrum in a weapon. We are collaborating with experimentalists using the GEANIE gamma-ray detector to determine this cross section in support of an enhanced nuclear test archival analysis capability. Calculations include fission, compound nucleus, preequilibrium, and direct reaction mechanisms and predict the gamma-ray cascades in the residual nucleus.

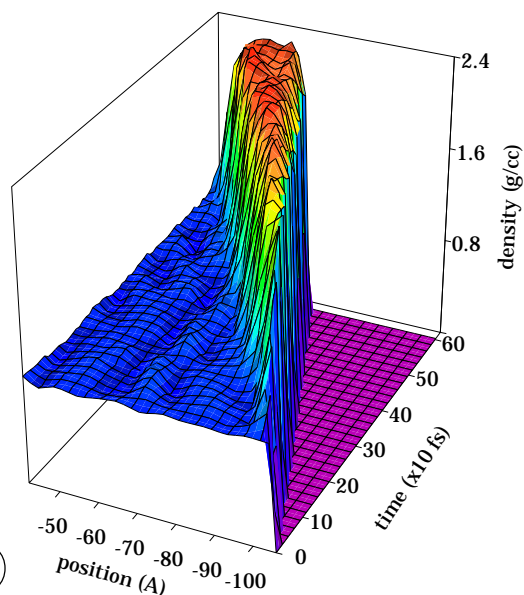
10



3D Computer Simulation of Loss of Circulation in 3-Phase Draft-Tube Bubble Columns

We use a finite-volume flow simulation technique to represent a three-phase flow in a conical-bottom draft-tube bubble column. To our knowledge, this work is the first reported calculation of a three-dimensional, three-phase bubble column of any kind. The simulations reproduced the qualitative experimentally-observed effects of draft-tube positioning on column circulation.

11



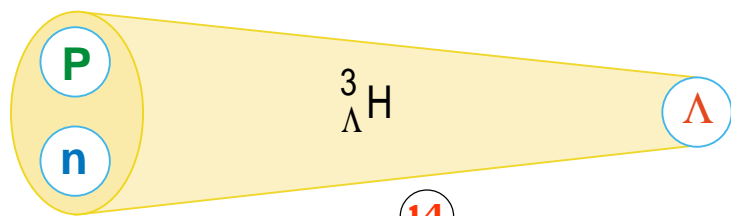
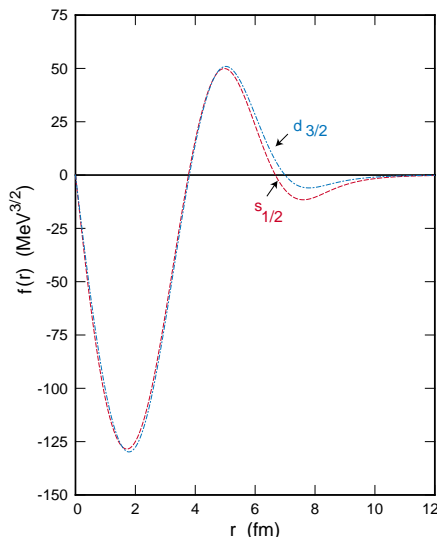
12

Simulations of Shock-Compressed Hydrocarbons: Nonequilibrium molecular dynamics simulations of large samples of hydrocarbons produce shock waves traveling through the medium. These shocks result in a dramatic increase in density and temperature in the material behind the front, leading to molecular dissociation and the formation of polymers and molecular hydrogen. In the figure, we follow the evolution of a shock front in time and space.

A Relativistic Symmetry

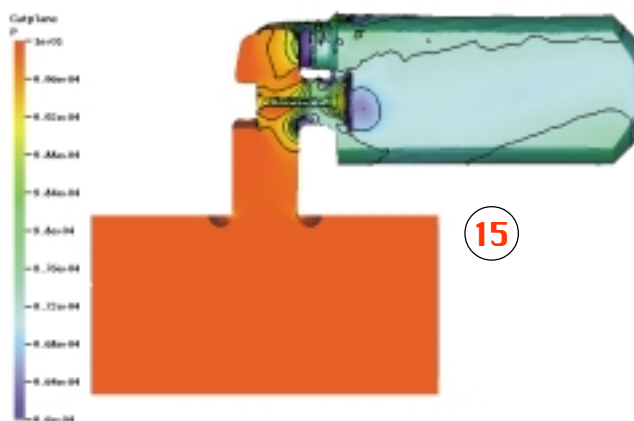
in Nuclei: Quasidegenerate pseudospin doublets in nuclei, discovered nearly 30 years ago, are now understood as resulting from a relativistic Hamiltonian in which the scalar and vector potentials are nearly equal, but opposite, and as a consequence of which the energies of the doublet are nearly equal and the lower components of the corresponding Dirac wave functions are almost identical.

13



14

Likely the World's Largest Halo Nucleus: Halo nuclei are characterized by nucleons tenuously bound to a compact core. A Λ , the lowest mass “strange” baryon, binds to the deuteron core with $\sim 2\%$ of the strength that a neutron binds to the deuteron core in a conventional triton. The Λ resides ~ 7 times as far from the deuteron as does the additional neutron in the triton.



Simulations of Diesel Engine Port Flow: Group T-3 and Caterpillar Inc. are collaborating on computer simulations of flows in diesel engine geometries. The valves are fixed at maximum lift, and the simulation includes the effects of turbulence on the solution. At steady state, the experimental and computed mass-flow rates agreed to within 1%. This work is supported by DOE's Office of Heavy Vehicle Technologies.

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